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NEW INSIGHTS IN THE PHOTOCHEMISTRY OF GRAIN MANTLES: THE IDENTIFICATION OF THE 4.62 AND 6.87 μm BANDS

by

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The mid-IR spectral region of molecular clouds is known to show the fingerprints of molecules frozen in the icy mantles of the interstellar grains. So far, only a few molecules have been positively identified: H_2O, CO, OCS, H_2S and CH_3OH. With the recent identification of the 4.62 μm absorption band in W33A with the OCN^- ion (Grim and Greenberg 1987) a new field of potential candidates became available. To study in more detail the complex chemical and physical interactions going on in the ice mantles accreted on grains in molecular clouds we performed numerous experiments involving UV irradiation and diffusion experiments. We present here some new ideas about the photochemistry of molecular ices, whereas the diffusion will be addressed in the paper by Schmitt *et al.*.

Although our ultimate aim was to study irradiated astrophysically relevant molecular ices for comparison with interstellar spectra, we have started our research with the irradiation of binary ices. Using isotopic labelling on NH_3/CO and NH_3/O_2 ices we have identified numerous compounds, of which the OCN^-, NO_2^-, NO_3^-, and NH_4^+ ions are the most interesting ones since they reveal a new type of chemical reactions. It appeared that these compounds were formed by proton transfer reactions induced by the interaction between an acid (HNCO, HNO_2, HNO_3) and a base (NH_3) through a hydrogen bond. This mechanism has been confirmed by a study of photolyzed diluted argon mixtures ($Ar/NH_3/CO$ and $Ar/NH_3/O_2$) that were allowed to anneal slowly, permitting the transfer reactions to occur. Using the collected data of these two particularly studies, we reached a better understanding of the effects of UV irradiation of such complex mixtures as $H_2O/NH_3/CO/O_2 = 10/1/1/1$.

The main astrophysically relevant results from the overall study are presented. Firstly, the 4.62 μm band in W33A can be reproduced with NH_3/CO containing irradiated ices and has been identified with OCN^- (Grim and Greenberg 1987). The 6.87 μm band in W33A and other protostellar objects is reproduced with NH_3/O_2 containing ices (Figure 1a) and is identified with NH_4^+.

For W33A the following column densities relative to H_2O have been calculated: $[OCN^-]/[H_2O] \sim 1\%$ and $[NH_4^+]/[H_2O] \sim 2\%$. The 5-8 μm spectrum of W33A shows significant line of sight effects. The 6.0 μm H_2O band is carried by grains that have a relatively low temperature, but the position of the 6.87 μm indicated grains that are heated to higher temperatures. The more complex 5-8 μm spectrum of Mon R2/IRS 2 shows three interesting regions (Figure 1b): (i) an absorption excess from 5.2 to 5.8 μm which is not understood yet, (ii) a very steep rise at 6.1 μm that constrains the maximum contribution of H_2O and requires the presence of other compounds to account for the observed 6.0 μm band, and (iii) the broad 6.87 μm band can not be explained solely by NH_4^+, but ammonium salts might explain the observed broadening.

References:

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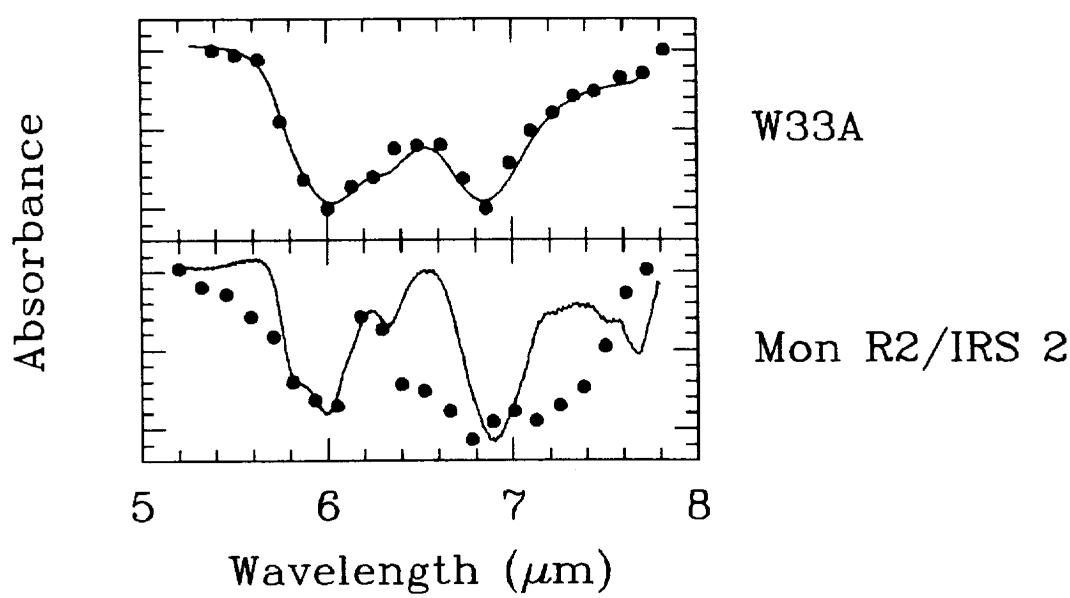

Figure 1: The 5-8 μm spectrum of W33A compared with $H_2O/NH_3/CO/O_2 = 10/1/1/1$ after UV irradiation and annealing to 176 K (a), and the 5-8 μm spectrum of Mon R2/IRS 2 compared with the same mixture but after sufficient time at 176 K to sublimate all H_2O (b). The observational data are taken from Tielens and Allamandola (1987).